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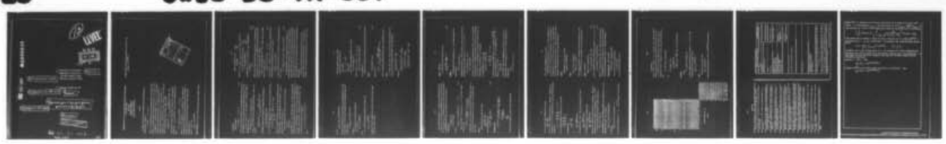

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1210 West Dayton Street
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(12) 17p.

(9) Technical rept.

TECHNICAL REPORT NO. 557

(14) UWIS-DS-TR-557

(11) March 1979

(6) CONVERGENCE RATES OF 'THIN PLATE' SMOOTHING SPLINES WHEN THE DATA ARE NOISY.

(15) N00014-77-C-0675

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CONVERGENCE RATES OF "THIN PLATE" SMOOTHING SPLINES WHEN THE DATA ARE NOISY

(Preliminary report)

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Abstract

We study the use of "thin plate" smoothing splines for smoothing noisy d dimensional data. The model is

$$z_i = u(t_i)+\epsilon_i , \qquad i = 1,2,\ldots,n ,$$

where u is a real valued function on a closed, bounded subset Ω of Euclidean d-space and the ϵ_i are random variables satisfying $E\epsilon_i=0$, $E\epsilon_i\epsilon_j=\sigma^2$, $i=j$, $=0$, $i\neq j$, $t_i\in\Omega$. The z_i are observed. It is desired to estimate u, given $z_1,\ldots,z_n$. u is only assumed to be "smooth", more precisely we assume that u is in the Sobolev space $H^m(\Omega)$ of functions with partial derivatives up to order m in $L_2(\Omega)$, with $m>d/2$. u is estimated by $u_{n,m,\lambda}$, the restriction to Ω of $\tilde{u}_{n,m,\lambda}$, where $\tilde{u}_{n,m,\lambda}$ is the solution to: Find $\tilde{u}$ (in an appropriate space of functions on R^d) to minimize

$$\frac{1}{n}\sum_{i=1}^{n}(\tilde{u}(t_i)-z_i)+\lambda\sum_{i_1,\ldots,i_m=1}^{d}\int_{R^d}\left(\frac{\partial^m\tilde{u}}{\partial x_{i_1}\partial x_{i_2}\cdots\partial x_{i_m}}\right)^2 dx_1,dx_2,\ldots,dx_d .$$

This minimization problem is known to have a solution for $\lambda>0$, $m>\frac{d}{2}$, $n\geq M=\binom{m+d-1}{d}$, provided the $t_1,\ldots,t_n$ are "unisolvent". We consider the integrated mean square error

$$R(\lambda) = \frac{1}{|\Omega|}\int_\Omega (u_{n,m,\lambda}(t)-u(t))^2dt , \qquad |\Omega| = \int_\Omega dt ,$$

and $ER(\lambda)$, as $\{t_i\}_{i=1}^n$ become dense in Ω. An estimate of λ which asymptotically minimizes $ER(\lambda)$ can be obtained by the method of generalized cross-validation. In this paper we give plausible arguments and numerical evidence supporting the following conjectures:

Suppose $u \in H^m(\Omega)$. Then

$$\min_\lambda ER(\lambda) = O(n^{-2m/(2m+d)}) .$$

Suppose $u\in H^{2m}(\Omega)$ and certain other conditions are satisfied. Then

$$\min_\lambda ER(\lambda) = O(n^{-4m/(4m+d)}) .$$

Research supported by the Office of Naval Research under Grant No. N00014-77-C-0675.

1. Introduction

Consider the model

$$z_i = u(t_i)+\epsilon_i\ , \qquad i = 1,2,\ldots,n \tag{1.1}$$

where u is some "smooth" function on Ω, a closed, bounded subset of R^d, and the $\{\epsilon_i\}$ are independent, zero mean random variables with common unknown variance σ^2. The $t_1,\ldots,t_n$ are in Ω, and $\underset{\sim}{z} = (z_1,\ldots,z_n)'$ is observed. It is desired to estimate u nonparametrically from $\underset{\sim}{z}$.

Our estimate $u_{n,m,\lambda}$ for u will be obtained as follows:

Let $\tilde{u}_{n,m,\lambda}$ be the solution the the following minimization problem: Find $\tilde{u} \in \underline{X}$ to minimize

$$\frac{1}{n}\sum_{i=1}^{n}(\tilde{u}(t_i)-z_i)^2+\lambda \sum_{i_1,\ldots,i_m=1}^{d} \int_{R_d} \left(\frac{\partial^m \tilde{u}}{\partial x_{i_1}\cdots\partial x_{i_m}}\right)^2 dx_1\ldots dx_d\ .$$

For example, when $d=2$, $m=2$, the second or "smoothness penalty" term becomes

$$\lambda \int_{R^2} (\tilde{u}^2_{x_1x_1}+2\tilde{u}^2_{x_1x_2}+\tilde{u}^2_{x_2x_2})dx_1dx_2\ ,$$

which is the bending energy of a thin plate. The space $\underline{X}$ is the "Beppo Levi" space

$$\underline{X} = \{\tilde{u}\in\mathcal{D}',\ \frac{\partial^{\alpha_1+\ldots+\alpha_d}\tilde{u}}{\partial x_1^{\alpha_1}\ldots\partial x_d^{\alpha_d}} \in L_2(R^d),\ \text{for } \alpha_1+\ldots+\alpha_d=m\}$$

where $\mathcal{D}'$ is the dual of the Schwartz space $\mathcal{D}$ of infinitely differentiable functions with compact support. See Meinguet (1978,1979) for further details. $u_{n,m,\lambda}$ is taken as the restriction of $\tilde{u}_{n,m,\lambda}$ to Ω.

A unique (continuous) solution is known to exist for any $\lambda>0$ provided

$$m > d/2$$

$$n \ge M = \binom{m+d-1}{d}$$

and the "design" $t_1,\ldots,t_n$ is "unisolvent", that is, if $\{\phi_\nu\}_{\nu=1}^{M}$ are a basis for the M dimensional space of polynomials of total degree $m-1$ or less, then $\sum_{\nu=1}^{M} a_\nu\phi_\nu(t_i) = 0$, $i = 1,2,\ldots,n$, implies that the a_ν are all 0. See Duchon (1976a,1976b), Meinguet (1978,1979), Paihua (1977,1978). We henceforth assume these conditions. Duchon has shown that the solution has a representation

$$\tilde{u}_{n,m,\lambda}(t) = \sum_{j=1}^{n} c_jE_m(t,t_j) + \sum_{\nu=1}^{M} d_\nu\phi_\nu(t)\ ,$$

where

$$E_m(s,t) = \theta_m|s-t|^{2m-d}\log|s-t| \qquad m \text{ even}$$
$$\qquad = \theta_m|s-t|^{2m-d} \qquad m \text{ odd}$$

where, if $s = (x_1,\ldots,x_d)$, $t = (y_1,\ldots,y_d)$, $|s-t| = (\sum_{i=1}^{d}(x_i-y_i)^2)^{1/2}$, and

$$\theta_m = (-1)^{d/2+1}/(2^{2m-1}\pi^{d/2}(m-1)!\,(m-d/2)!) \qquad m \text{ even}$$
$$\quad = (-1)^m\Gamma(d/2-m)/2^{2m}\pi^{d/2}(m-1)! \qquad m \text{ odd}\ .$$

The coefficients $\underset{\sim}{c} = (c_1,\ldots,c_n)'$ and $\underset{\sim}{d} = (d_1,\ldots,d_M)'$ are determined by

$$(K+\rho I)\underset{\sim}{c}+T\underset{\sim}{d} = \underset{\sim}{z} \tag{1.2}$$

$$T'\underset{\sim}{c} = 0\ , \tag{1.3}$$

where K is the $n\times n$ matrix with jk^{th} entry $E_m(t_j,t_k)$, $\rho=n\lambda$, T is the $n\times M$ matrix with $i\nu^{th}$ entry $\phi_\nu(t_i)$ and $\underset{\sim}{z} = (z_1,\ldots,z_n)'$. See Duchon (1976,1977), Paihua (1977,1978), Wahba (1979). We discuss the choice of λ shortly.

Let Ω be a closed, bounded subset in R^d. We will suppose that the $\{t_i\}$ become dense in Ω in such a way that

$$\lim \frac{1}{n}\sum_{i=1}^{n}\rho(t_i) = \frac{1}{|\Omega|}\int_\Omega \rho(t)dt\ , \qquad |\Omega| = \int_\Omega dt \tag{1.4}$$

for any continuous ρ. (However, it will be clear that our rate arguments hold under weaker conditions on the distribution of the $\{t_i\}$, for example

$$\lim \frac{1}{n}\sum_{i=1}^{n}\rho(t_i) = \int_\Omega \rho(t)w(t)dt$$

for some sufficiently nice positive w.) Let $R(\lambda)$ be the integrated mean square error when λ is used:

$$R(\lambda) = \frac{1}{n}\sum_{i=1}^{n}(u_{n,m,\lambda}(t_i)-u(t_i))^2 \approx \frac{1}{|\Omega|}\int_\Omega (u_{n,m,\lambda}(t)-u(t))^2dt\ . \tag{1.5}$$

The smoothing parameter λ^* which minimizes $ER(\lambda)$ can be estimated by the method of generalized cross-validation (GCV), see Craven and Wahba (1979), Golub, Heath and Wahba (1977), Wahba (1979). Pleasing numerical results have been obtained in Monte Carlo studies for $d=1$, $m=2$ (Craven and Wahba (1979)) and $d=2$, $m=2$, Wahba (1979). Convergence rates for $ER(\lambda^*)$ have been obtained in the one dimensional case (Wahba (1975)).

Stone (1978) has recently obtained some rather general results on best achieveable pointwise convergence rates for the model (1.1), for any method of estimation of $u(t)$. Reduced to our case and phrased loosely, his results say that

the rate

$$E(\tilde{u}(t)-u(t))^2 = O(n^{-(2m-1)/(2m-1+d)}) ,$$

where $\tilde{u}(t)$ is any estimate of $u(t)$ from the data $\underset{\sim}{z}$, can be achieved for all $u \in H_m(\Omega)$ but not bettered. In this paper we are concerned with integrated mean square error convergence rates: —

$$E \frac{1}{|\Omega|} \int_\Omega (u_{n,m,\lambda^*}(t)-u(t))^2 dt = ER(\lambda^*)$$

of u_{n,m,λ^*}.

It is our goal to give a plausible argument that

i) if $u \in H^m(\Omega)$,

$$ER(\lambda^*) = O(n^{-2m/(2m+d)})$$

and if

ii) $u \in H^{2m}(\Omega)$ and some other conditions are satisfied, then

$$ER(\lambda^*) = O(n^{-4m/(4m+d)})$$

Our argument follows the arguments given in Wahba (1975,1977) and Craven and Wahba (1979), and is given in section 2.

2. Plausibility arguments, numerical evidence

Let $A(\lambda)$ be the $n \times n$ matrix defined by

$$\begin{pmatrix} u_{n,m,\lambda}(t_1) \\ \vdots \\ u_{n,m,\lambda}(t_n) \end{pmatrix} = A(\lambda)\underset{\sim}{z} .$$

If $R(\lambda)$ is taken as the middle quantity in (1.5), we have

$$R(\lambda) = \frac{1}{n} ||A(\lambda)(\underset{\sim}{u}+\underset{\sim}{\varepsilon})-\underset{\sim}{u}||^2$$

where $\underset{\sim}{u} = (u(t_1),\dots,u(t_n))'$, $\underset{\sim}{\varepsilon} = (\varepsilon_1,\dots,\varepsilon_n)'$, and

$$ER(\lambda) = \frac{1}{n} ||(I-A(\lambda))\underset{\sim}{u}||^2 + \frac{\sigma^2}{n} \text{Trace } A^2(\lambda) . \tag{2.1}$$

($A(\lambda)$ is symmetric.)

We call $\frac{1}{n} ||(I-A(\lambda))\underset{\sim}{u}||^2$ the "squared bias" and (σ^2/n) Trace $A^2(\lambda)$ the variance.

<u>Lemma 1</u>.

$$\frac{1}{n} ||(I-A(\lambda))\underset{\sim}{u}||^2 \le \lambda J_m(\tilde{u}) \tag{2.2}$$

where, for $\tilde{v} \in \underline{X}$

$$J_m(\tilde{v}) = \sum_{i_1,\dots,i_m=1}^{d} \int_{R^d} \left(\frac{\partial^m \tilde{v}(x_1,\dots,x_d)}{\partial x_{i_1}\dots\partial x_{i_m}}\right)^2 dx_1\dots dx_m$$

and $\tilde{u}$ is that element in $\underline{X}$ which minimizes J_m subject to coinciding with u on Ω.

<u>Proof</u>.

For each i, $\tilde{u}(t_i) = u(t_i)$. $A(\lambda)\underset{\sim}{u}$ is a vector of values of the function, call it $\tilde{u}^*_{n,m,\lambda}$ which is the solution to the problem: Find $\tilde{v} \in \underline{X}$ to minimize

$$\frac{1}{n} \sum_{j=1}^{n} (u(t_j)-\tilde{v}(t_j))^2 + \lambda J_m(\tilde{v}) .$$

Therefore

$$\frac{1}{n} \sum_{j=1}^{n} (u(t_j)-\tilde{u}^*_{n,m,\lambda}(t_j))^2 + \lambda J_m(\tilde{u}^*_{n,m,\lambda})$$

$$= \frac{1}{n} ||(I-A)\underset{\sim}{u}||^2 + \lambda J_m(\tilde{u}^*_{n,m,\lambda})$$

$$\le \frac{1}{n} \sum_{j=1}^{n} (u(t_j)-\tilde{u}(t_j))^2 + \lambda J_m(\tilde{u}) = \lambda J_m(\tilde{u}) .$$

We now investigate Trace $A^2(\lambda)$. Let $T_{n\times M}$ be the $n\times M$ dimensional matrix with $j\nu^{th}$ entry $\phi_\nu(t_j)$. Let R by any $n\times(n-M)$ dimensional matrix of rank $n-M$ satisfying $R'T = 0_{(n-M)\times M}$, $R'R = I_{n-M}$. Following the results of Anselone and Laurent (1968) it is shown in Wahba (1979) that $\underset{\sim}{c}$ and $\underset{\sim}{d}$ satisfying (1.2) and (1.3) have the representations

$$\underset{\sim}{c} = R(R'KR+\rho I)^{-1}R'\underset{\sim}{z}$$

$$\underset{\sim}{d} = (T'T)^{-1}T'(\underset{\sim}{z}-K\underset{\sim}{c})$$

and that

$$(I-A(\lambda))\underset{\sim}{z} = \rho\underset{\sim}{c} = n\lambda R(R'KR+n\lambda I)^{-1}R'\underset{\sim}{z}\,, \qquad \underset{\sim}{z} \in E_n\,. \tag{2.3}$$

Hence, if we define $B = R'KR$ and let $b_{\nu n}$, $\nu = 1,2,\ldots,n-M$ be the $n-M$ eigenvalues of B, then

$$\frac{1}{n}\,\mathrm{Tr}\,A^2(\lambda) = \frac{1}{n}\sum_{\nu=1}^{n}\left(\frac{b_{\nu n}}{b_{\nu n}+n\lambda}\right)^2 = \frac{1}{n}\sum_{\nu=1}^{n}\frac{1}{(1+n\lambda/b_{\nu n})^2}\,.$$

We remark that K is not, in general, positive definite, however R'KR is, since it is known that $\underset{\sim}{r}'K\underset{\sim}{r}>0$ for any non-trivial $\underset{\sim}{r}$ satisfying $T'\underset{\sim}{r} = 0$ (See Paihua (1977), Duchon (1977)).

<u>Lemma 2</u>.

Suppose there exist $p>1$, and $k_1>0$ such that

$$\lim_{\nu\to\infty}\lim_{n\to\infty}\left|\frac{b_{\nu n}}{n} - \frac{k_1}{\nu^p}\right| \to 0$$

then, for some constant k_2,

$$\frac{1}{n}\,\mathrm{Tr}\,A^2(\lambda) = \frac{k_2}{n\lambda^{1/p}}(1+o(1))\,. \tag{2.4}$$

<u>Outline of Proof</u>.

$$\frac{1}{n}\,\mathrm{Tr}\,A^2(\lambda) = \frac{1}{n}\sum_{\nu=1}^{n}\frac{1}{(1+\lambda n/b_{\nu n})} \approx \frac{1}{n}\sum_{\nu=1}^{n}\frac{1}{(1+k_1^{-1}\lambda\nu^p)^2}$$

$$\approx \frac{1}{n}\int_0^\infty \frac{dx}{(1+k_1^{-1}\lambda x^p)^2}$$

$$= \frac{k_2}{n\lambda^{1/p}}$$

(A more rigorous argument can be found in Craven and Wahba 1979)).

<u>Lemma 3</u>. (Conjecture)

For $2m/d>1$ there exists a constant k such that

$$\lim_{\nu\to\infty}\left(\lim_{n\to\infty}\left|\frac{b_{\nu n}}{n} - \frac{k}{\nu^{2m/d}}\right|\right) = 0\,. \tag{2.5}$$

<u>Argument</u>

We first argue that the eigenvalues $\lambda_1,\lambda_2,\ldots$ of the integral operator K on $L_2(\Omega)$ defined by

$$(Ku)(t) = \int_\Omega E_m(t,s)u(s)ds$$

asymptotically behave like $\lambda_\nu = k/\nu^{2m/d}$, for some k, and then that this entails that the eigenvalues $b_{\nu n}$ of K behave like $n\lambda_\nu/|\Omega|$, $\nu = 1,2,\ldots,n$, $n = 1,2,\ldots$.

Δ^m is a left inverse of K, since, if

$$\psi(t) = \int_\Omega E_m(t,s)\phi(s)ds$$

then $\Delta^m\psi(t) = \phi(t)$, $t\in\Omega$ (See Courant and Hilbert (1953)). Thus it is to be expected that the eigenvalues of K asymptotically decrease at the same rate as the eigenvalues of Δ^m increase. Let $d = 2$ and suppose Ω is the rectangle with sides a_1 and a_2. The eigenfunctions $\{\phi\}$ and eigenvalues $\{\rho\}$ for the equation

$$\Delta u = \rho u$$

with boundary conditions $u = 0$ on $\partial\Omega$ are

$$\phi_{\xi,\eta}(x_1,x_2) = \sin\frac{\xi\pi x_1}{a_1}\sin\frac{\eta\pi x_2}{a_2}$$

$$\rho_{\xi\eta} = \pi^2\left(\frac{\xi^2}{a_1^2}+\frac{\eta^2}{a_2^2}\right)\,, \qquad \xi,\eta = 1,2,\ldots$$

It follows, by counting the number of pairs (ξ,η) in the ellipse $\pi^2\left(\frac{x_1^2}{a_1^2}+\frac{x_2^2}{a_2^2}\right) \le c$, that, if the eigenvalues $\rho_{\xi\eta}$ $(\xi,\eta = 1,2,\ldots)$ are reindexed in size place as ρ_ν, $\nu = 1,2,\ldots$ that

$$\lim_{\nu\to\infty}\frac{\rho_\nu}{\nu} = \frac{4\pi}{|\Omega|}\,.$$

This relation is known to hold independently of the shape of Ω, and also for a Neumann boundary condition instead of $u = 0$ on $\partial\Omega$. Similarly eigenfunctions and eigenvalues for

$$\Delta^m u = \rho u$$

$$\Delta^k u = 0 \text{ on } \partial\Omega,\ k = 0,1,\ldots,m-1$$

are $\phi_{\xi,\eta}$ and $\rho^m_{\xi\eta}$ so that the eigenvalues (ρ_ν) satisfy

$$\lim_{\nu\to\infty} \frac{\rho_\nu}{\nu^m} = \left(\frac{4\pi}{|\Omega|}\right)^m ,$$

and this result is independent of the shape of Ω. Going to $d = 3$ dimensions, the eigenvalues for $\Delta u = \rho u$ on a rectangle with sides a_1, a_2 and a_3 and suitable boundary conditions are

$$\rho_{\xi,\eta,\psi} = \pi^2 \left(\frac{\xi^2}{a_1^2} + \frac{\eta^2}{a_2^2} + \frac{\psi^2}{a_3^2}\right) \qquad \xi,\eta,\psi = 1,2,\ldots$$

and, by counting the number of triplets (ξ,η,ψ) in the ellipse

$$\pi^2 \left(\frac{x_1^2}{a_1^2} + \frac{x_2^2}{a_2^2} + \frac{x_3^2}{a_3^2}\right) \le c$$

one obtains that

$$\lim_{\nu\to\infty} \frac{\rho_\nu^{3/2}}{\nu} = \frac{6\pi^2}{|\Omega|} .$$

or

$$\frac{\rho_\nu}{\nu^{2/3}} = \left(\frac{6\pi^2}{|\Omega|}\right)^{2/3}(1+o(1)) .$$

See Courant and Hilbert (1953). Similarly the eigenvalues for Δ^m satisfy

$$\frac{\rho_\nu}{\nu^{2m/3}} = \left(\frac{6\pi^2}{|\Omega|}\right)^{2m/3}(1+o(1))$$

and, extending the argument to d dimensions gives

$$\frac{c_\nu}{\nu^{2m/d}} = \left(\frac{(2\pi)^d}{V_d|\Omega|}\right)^{2m/d}(1+o(1))$$

where V_d is the volume of the sphere of radius 1 in d dimensions. Therefore, we conjecture that the rate of decrease of the eigenvalues (λ_ν) of K is $\nu^{-2m/d}$.

Let $K(s,t)$ be a kernel with a Mercer-Hilbert Schmidt expansion on Ω,

$$K(s,t) = \sum_{\nu=1}^{\infty} \lambda_\nu \phi_\nu(s)\phi_\nu(t)$$

where the eigenvalues (λ_ν) are absolutely summable and the eigenfunctions (ϕ_ν) are an orthonormal set on $L_2(\Omega)$. Then, for large n,

$$K(t_i,t_j) \simeq \sum_{\nu=1}^{n} n\lambda_\nu(\phi_\nu(t_i)/\sqrt{n})(\phi_\nu(t_j)/\sqrt{n}) ,$$

and provided

$$\frac{|\Omega|}{n}\sum_{i=1}^{n} \phi_\nu(t_i)\phi_\mu(t_i) \simeq \int_\Omega \phi_\nu(t)\phi_\mu(t)dt = 1,\ \mu = \nu$$
$$= 0,\ \mu \ne \nu ,$$

we see that the eigenvalues $\lambda_{\nu n}$, $\nu = 1,2,\ldots,n$, say, of the matrix K with jk^{th} entry

$K(t_j,t_k)$, have an approximation as $\lambda_{\nu n} \sim n\lambda_\nu/|\Omega|$.

We have computed the eigenvalues $b_{\nu n}$, $\nu = 1,2,\ldots,n-M$ for an example with $d = 2$, $m = 2$, and $n = 81$. Thus there are $n-M = 78$ eigenvalues. The t_i are arranged on a 9×9 square array. If $b_{\nu n} \sim c\nu^{-p}$, then a plot of $b_{\nu n}$ vs. ν on log-log paper should fall on a straight line with slope $-p$, here $p = 2$. Figure 1 gives a plot of these 78 eigenvalues. For comparison, a solid line has been drawn with slope -2.

<u>Theorem</u>

Suppose Lemma 3 is true. Then, if $u \in H^m(\Omega)$,

$$\min_\lambda ER(\lambda) = O(n^{-2m/(2m+d)}) .$$

<u>Proof</u>

By (2.1), (2.2), (2.4) and (2.5)

$$ER(\lambda) \le c_1\lambda + c_2/n\lambda^{d/2m}$$

where c_1 and c_2 are constants. Minimizing this expression with respect to λ gives $\lambda^* = O(n^{-2m/(2m+d)})$, where λ^* is the minimizer of $R(\lambda)$, and thence the result.

<u>Lemma 4</u>. (Conjecture)

Suppose u has a representation

$$u(t) = \int_\Omega E_m(t,s)\rho(s)ds + \sum_{\nu=1}^{M} \theta_\nu\phi_\nu(t) \qquad (2.6)$$

where ρ is piecewise continuous and satisfies $\int_\Omega \phi_\nu(s)\rho(s)ds = 0$, $\nu = 1,2,\ldots,M$. Then

$$\frac{1}{n}\,||(I-A(\lambda))\underset{\sim}{u}||^2 \le \lambda^2\,|\Omega|\int_\Omega (\Delta^m u)^2 dt(1+o(1)) . \qquad (2.7)$$

Remark: If u has the given form, then $\rho = \Delta^m u$. However, the class of functions with representation (2.6) is restrictive since, for example it excludes harmonic functions other than polynomials of degree $\le m$. (See Courant and Hilbert)

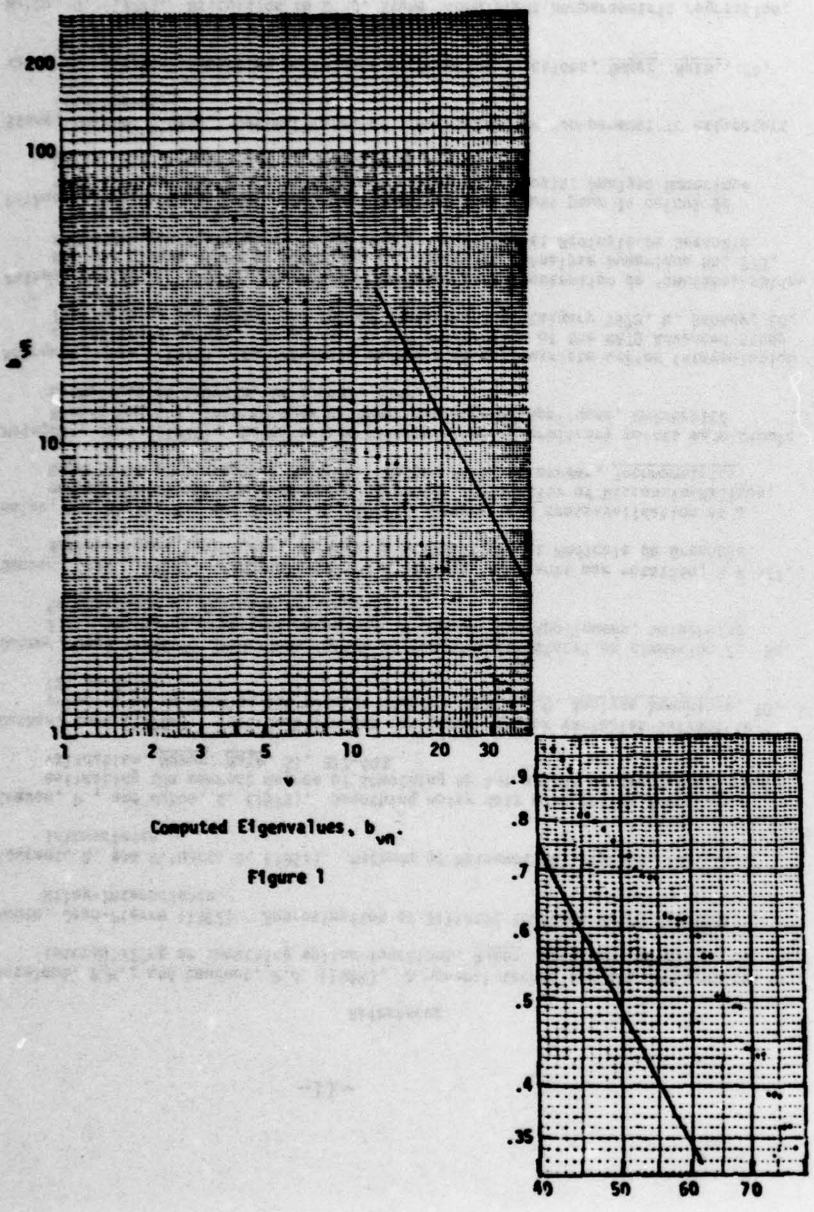
<u>Suggestion of proof</u>. From (2.3) we have

$$\frac{1}{n}\,||(I-A(\lambda))\underset{\sim}{u}||^2 = n\lambda^2\underset{\sim}{u}'R(RKR'+n\lambda I)^{-2}R'\underset{\sim}{u}$$

and the right hand side is bounded above by

$$n\lambda^2\,||(RKR')^{-1}R'\underset{\sim}{u}||^2$$

If u has the required form (2.6), then



Computed Eigenvalues, $b_{\nu m}$.

Figure 1

$$\underset{\sim}{u} = \frac{|\Omega|}{n} K\underset{\sim}{\rho} + T\underset{\sim}{\theta} + \underset{\sim}{\delta}^1$$

where $\underset{\sim}{\rho} = (\rho(t_1),\ldots,\rho(t_n))'$, $\underset{\sim}{\theta} = (\theta_1,\ldots,\theta_M)'$ and $\underset{\sim}{\delta}' = (\delta_1^1,\ldots,\delta_n^1)$ is a vector of quadrature errors which we must assume are negligible in the limit. Similarly $T'\underset{\sim}{\rho} = \underset{\sim}{\delta}^2$, where δ^2 is a vector of quadrature errors which we must assume are negligible in the limit. Assuming $T'\underset{\sim}{\rho} = 0$, then $\underset{\sim}{\rho} = R\underset{\sim}{\rho}_0$, for some n-M vector ρ_0.

Then

$$R'\underset{\sim}{u} = \frac{|\Omega|}{n} R'KR\underset{\sim}{\rho}_0 + \text{negligible terms}$$

and

$$n\lambda^2 \underset{\sim}{u}'R(RKR'+n\lambda I)^{-2}R'\underset{\sim}{u}$$

$$\leq n\lambda^2 \underset{\sim}{u}'R(RKR')^{-2}R'\underset{\sim}{u}$$

$$= \frac{\lambda^2|\Omega|^2}{n} ||\underset{\sim}{\rho}_0||^2 = \frac{\lambda^2|\Omega|^2}{n} ||\underset{\sim}{\rho}||^2 = \lambda^2|\Omega| \int_\Omega \rho^2(t)dt(1+o(1)) .$$

__Theorem 2.__

Suppose

$$u(t) = \int_\Omega E_m(t,s)\rho(s)ds + \sum_{\nu=1}^{M} \theta_\nu \phi_\nu(t)$$

for some ρ piecewise continuous with $\int_\Omega \phi_\nu(s)\rho(s)ds = 0$, $\nu = 1,2,\ldots,M$. Then (assuming the conclusions of lemmas 3 and 4),

$$\min_\lambda R(\lambda) = O(n^{-4m/(4m+d)})$$

__Proof.__

Using (2.4), (2.5) and (2.7) gives

$$R(\lambda) \leq k_3\lambda^2 + k_4/n\lambda^{d/2m}$$

where k_3 and k_4 are constants. Setting $\lambda = O(n^{-2m/(4m+d)})$ gives the result.

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER ✓ TR#557	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) ✓ CONVERGENCE RATES OF "THIN PLATE" SMOOTHING SPLINES WHEN THE DATA ARE NOISY		5. TYPE OF REPORT & PERIOD COVERED
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Grace Wahba		8. CONTRACT OR GRANT NUMBER(s) ✓ ONR # N00014-77-C-0675
9. PERFORMING ORGANIZATION NAME AND ADDRESS ✓ Department of Statistics, University of Wisconsin, Madison, Wisconsin 53706		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research, 800 N. Quincy Street, Arlington, VA 22217		12. REPORT DATE March 1979
		13. NUMBER OF PAGES 13
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Distribution of this document is unlimited

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

multidimensional spline smoothing
generalized cross validation
surface smoothing

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

We study the use of "thin plate" smoothing splines for smoothing noisy d dimensional data. The model is

$$z_i = u(t_i)+\epsilon_i, \quad i = 1,2,\ldots,n ,$$

where u is a real valued function on a closed, bounded subset Ω of Euclidean d-space and the ϵ_i are random variables satisfying $E\epsilon_i=0$, $E\epsilon_i\epsilon_j=\sigma^2$, $i=j$, $=0$, $i\neq j$, $t_i\epsilon\Omega$. The z_i are observed. It is desired to estimate u, given $z_1,\ldots,z_n$. u is only assumed to be "smooth", more precisely we assume that u is in the Sobolev

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space $H^m(\Omega)$ of functions with partial derivatives up to order m in $L_2(\Omega)$, with $m>d/2$. u is estimated by $u_{n,m,\lambda}$, the restriction to Ω of $\tilde{u}_{n,m,\lambda}$, where $\tilde{u}_{n,m,\lambda}$ is the solution to: Find $\tilde{u}$ (in an appropriate space of functions on R^d) to minimize

$$\frac{1}{n}\sum_{i=1}^{n}(\tilde{u}(t_i)-z_i)+\lambda\sum_{i_1,\ldots,i_m=1}^{d}\int_{R^d}\left(\frac{\partial^m\tilde{u}}{\partial x_{i_1}\partial x_{i_2}\cdots\partial x_{i_m}}\right)^2 dx_1,dx_2,\ldots dx_d .$$

This minimization problem is known to have a solution for $\lambda>0$, $m>\frac{d}{2}$, $n\geq M\binom{m+d-1}{d}$, provided the $t_1,\ldots,t_n$ are "unisolvent". We consider the integrated mean square error

$$R(\lambda)=\frac{1}{|\Omega|}\int_\Omega (u_{n,m,\lambda}(t)-u(t))^2dt , \qquad |\Omega|=\int_\Omega dt ,$$

and $ER(\lambda)$, as $\{t_i\}_{i=1}^n$ become dense in Ω. An estimate of λ which asymptotically minimizes $ER(\lambda)$ can be obtained by the method of generalized cross-validation. In this paper we give plausible arguments and numerical evidence supporting the following conjectures:

Suppose $u \in H^m(\Omega)$. Then

$$\min_\lambda ER(\lambda) = O(n^{-2m/(2m+d)}) .$$

Suppose $u\in H^{2m}(\Omega)$ and certain other conditions are satisfied. Then

$$\min_\lambda ER(\lambda) = O(n^{-4m/(4m+d)}).$$